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On Using 'Emerging Interest' in Scientific Literature to Inform Chemical Risk Prioritisation

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Abstract: Modern industrial practices employ a large and diverse collection of chemicals. This can challenge regulators charged with environmental protection. Typically, insufficient data is available for risk assessments. Thus, chemicals may find widespread use until adequate evidence of adverse environmental effects prompts regulatory action. Globally, regulators have seen that such 'reactive' risk management has disadvantages. Recently in Australia (and elsewhere), relatively rapidly, certain unrestricted, long-used per- and polyfluoroalkyl substances (PFAS) became subjects of concern, then regulation. Such events motivate us to support regulators' 'proactive' risk management efforts. We aim to assist regulators in anticipating the emergence of potentially risky chemicals, enabling their timely actions. We hypothesise that a time series of research interest mined from a scientific publication database may reveal 'emerging interest' in a chemical that foreshadows its progress towards regulation. We investigate this for six PFAS by determining the associated research interest in Web of Science. For each chemical, we use R code to apply queries to an application programming interface, and count annual positive results across a publication year range. Inspection of these time series suggests two tests, each of which determines the first year in which some condition is satisfied. We propose classification rules to interpret test outcomes, and compare results against PFAS regulatory histories. For the regulated PFAS, we anticipate the historical progression of Australian regulatory concern. We also judge some unrestricted PFAS as being of concern, and this is validated by interest from other jurisdictions. These results demonstrate our system's predictive ability, and encourage further development.

Keywords: chemical regulation; classification; data mining; time series analysis.

1 INTRODUCTION

Modern industrial practices employ a large and diverse volume of chemicals. This is shown by a public inventory of over 40 000 chemicals available for Australian industrial use (National Industrial Chemicals Notification and Assessment Scheme, n.d.). Growth in chemical use has increased the demands on regulators charged with protecting environmental health. Typically the amount of data available for risk assessments is inadequate. Furthermore, a regulator's interest in a chemical may not end with a thorough assessment; new information may require consideration. However, the volume of chemicals requiring attention, coupled with limited resources, may delay a regulator's preparation (or revision) of a risk assessment. As such, harmful chemicals may enter into widespread use, remaining there until sufficient evidence of harm prompts (or enables) regulatory action. Such a 'reactive' approach to risk management has disadvantages.

We may demonstrate these with an example of global significance that we explore largely through the Australian regulatory context. In the recent past, certain long-used per- and polyfluoroalkyl substances (PFAS) progressed relatively rapidly from unrestricted use, to being of concern, to a "regulated" status. Consequences of this progression included elevated health concerns, forced chemical substitutions, and costly interruptions to major infrastructure projects due to concerns around how to dispose of contaminated soil (Jacks and Hatch, 2020). Whilst researchers have assayed the properties and effects of some well-known PFAS (such as PFOS and PFOA) in recent years, these are exceptions to a general trend:

> The majority of the many thousands of PFAS, including those in commercial use, have very limited or no toxicity data. This is a critical data gap in health effects information for PFAS. (Interstate Technology & Regulatory Council, PFAS Team, 2020, Page 97)

Inadequate data inhibits a regulator's ability to recognise chemicals likely to pose risks to environmental health, limiting its ability to act 'proactively' to reduce such risks. However, suppose that, even without toxicity data, a regulator could anticipate which chemicals are likely to emerge as causing adverse environmental effects. Then, the regulator could focus its efforts on assessing these chemicals, regulating those recognised as causing adverse effects. We hypothesise that the scientific research interest associated with a chemical over time may reveal 'emerging interest' in its associated harmfulness. Then, an analysis of data mined from a scientific publication database may allow us to recognise Chemicals of Interest (CoI) which are deserving of regulatory attention. We can validate our methodology by checking if our results can foreshadow the emergence of some 'test case' CoI associated with adverse effects.

In order to pursue this, we require a means of quantifying scientific research interest. We choose to apply different types of queries to a publication database. We refer to any publication which matches a query as a 'hit'. For each chemical we consider, we obtain the counts of hits in each publication year across a range of years. That is, for each chemical and type of query, we obtain a time series of hits.

We consider the time series of hits for a selection of six PFAS; a regulator has classified each as being of concern, or otherwise. We use these series in developing two 'classification systems', and apply these to each series individually. A system consists of two parts. The first is a set of tests for emerging interest. Each test is associated with an outcome: the year in which the test is first satisfied, or a non-result otherwise. The second part is a 'classification rule' that combines outcomes in classifying a chemical. We experimented with our system to produce one that reliably classifies chemicals. Such reliability gives us some confidence that further development of our system may yield one able to correctly classify chemicals of unknown harmfulness.

Our task is complicated by the modest number of classifications available for PFAS. Some were compiled by The Australian Government's National Industrial Chemicals Notification and Assessment Scheme (NICNAS). Where necessary, we also draw on other regulators' assessments.

The remainder of this paper is organised as follows. In Section 2 we introduce our methodology for obtaining research interest from a database of scientific publications, and present the PFAS we consider. We show the associated research interest time series, and draw on this in outlining the classification systems we apply to the data subsequently. Section 3 shows our classification results, and offers comment. Section 4 draws conclusions, and notes promising future directions.

2 PRELIMINARIES

Our methodology substantially extends that of a study (Whyte and Robinson, 2020) undertaken for the New South Wales Environment Protection Authority (NSW EPA). We require two sources of data: a database of scientific publications, and a collection of alternative chemical names and identifiers ('synonyms') to inform database queries. We begin with a consideration of features of data sources that led to their selection. We proceed to outline the types of queries applied to our chosen database, and present the selected PFAS and associated research interest data. We draw on features of this data in proposing our classification system.

2.1 Selection of Data Sources

Querying an online database via a web browser seems impractical. This approach is likely to produce errors, and be extremely time consuming when considering a large number of chemicals, especially those having many synonyms. These limitations would be magnified if it were necessary to repeat queries due to the appearance of new synonyms, or in order to update our estimates of research interest over time. Thus, in the interests of efficiency and reproducibility, we choose to consider a database that has an application program interface (API). An API allows us to obtain information via data mining, achieved here via R computer code (R Core Team, 2019).

For various reasons, Clarivate's Web of Science (WoS) presented as a suitable data source. This study accessed the WoS "API Lite". Other useful WoS features include:

- A "Topic Search", allowing simultaneous searching of the publication record fields: "Title", "Abstract", "Keywords" (supplied by the author(s)), and "Keywords Plus" (which has content "…supplied by an algorithm that provides expanded terms stemming from the record's cited references or bibliography", Clarivate (2020a)).
- A flexible syntax for composing queries. For example, WoS allows a Topic Search to contain a query such as "term1 NEAR/n term2", which finds any occurrences of term1 within n words of term2. This allows us to impose restrictions (explained in Section 2.2) on the results returned.

Regarding a source of chemical synonyms, we sought certain features. Broad coverage of both common names and systematic names (as in standard classification systems) is appropriate. Also required are the Chemical Abstracts Service Registry Number® (CASRN), and any associated "Alternate" or "Deleted" CASRNs. We ascertained that SciFinder® (Chemical Abstracts Service (2019), for a description of features, see American Chemical Society (2020)) was a suitable source of information. SciFinder® includes the "CAS Registry", which we may access by entering a name into the "Substance Identifier" function. However, SciFinder® limits us to obtaining information via a web browser. One must then manually transfer information to an input file which is employed in the subsequent data mining. This is not ideal. Yet, as we considered only six chemicals, the amount of necessary manual processing was limited.

2.2 Features of Queries Applied to Web of Science

Any individual query used in this study relates only to one particular chemical. We considered two types of queries, the second capable of greater selectivity than the first. A comparison of results obtained for our test case chemicals allows us to judge the usefulness of this selectivity.
Each query applied to WoS was composed of multiple conditions. We define a 'hit' as a publication which satisfies all conditions of a query. The simplest query type aims to determine 'total-hits' for a chemical under investigation. The component conditions of the query (combined with AND) are:

C1 a Topic Search for all chemical synonyms in a list drawn from SciFinder® (combined with OR; a publication is retained as a possible hit if the search finds at least one synonym),
C2 a search of the "Publication Year" field for some value in the range from 1989–2019, inclusive.

We note that total-hits may include 'unsuitable' publications that are unrelated to an adverse environmental effect. As such, total-hits may be an inappropriate measure of research interest in some situations. To address this, we also employ a query (to determine 'near-hits') that includes conditions (due to 'modifiers') in a WoS Topic Search. These modifiers (presented in Table 1) are intended to relate to adverse effects.

Table 1: Modifiers employed in queries intending to return near-hits. A $*$ denotes a 'wild card' operator. To demonstrate its use, a query using $*$ appended to a root, such as "*carcinogen*$*$", in a Topic Search seeks variants including *carcinogen*ic and *carcinogen*s. However, words having characters before the root, such as non*carcinogen*ic, are excluded from the search.

carcinogen$*$	dangerous$*$	ecotoxic$*$	fatal$*$	harmful$*$	hazardous$*$
injurious	lethal$*$	noxious$*$	poison$*$	toxic$*$	unsafe

That is, a query relating to near-hits returns the count of any hits satisfying conditions C1, C2, and:

C3 at least one modifier occurred at most three words from a synonym.

2.3 PFAS Considered in this Pilot Study

Various factors influenced the choice of PFAS to consider in this study. Initially we noted an Environmental Working Group report from the United States of America (Evans et al., 2020). The reported study tested tap water for a selection of 30 PFAS at 44 sites across 31 states and the District of Columbia. Results were collected between May and December 2019. The report's appendix noted the frequency of occurrence of PFAS across the sites. This suggested value in considering a selection of the most commonly occurring PFAS. Of these, we selected some PFAS of specific interest to NSW EPA contacts, and some others of no particular interest. Selection was guided by the need to include some PFAS for which there was a NICNAS environmental assessment. Table 2 shows a summary of identifiers associated with the selected PFAS.

Figure 1 presents the time series of annual counts of total-hits and near-hits for our PFAS. As we might expect, considering the results for any particular chemical, the near-hits value for a given year is typically smaller than the corresponding total-hits value. However, results for three chemicals show almost no near-hits. Such low values could be an accurate indicator of a general lack of concern in the scientific literature. Alternatively, this could indicate that our near-hits queries are unable to capture the relevant research interest, and we should see a greater proportion of the total-hits returned as near-hits. We will review our modifiers in a future study, and proceed here to use total-hits as our measure of research interest. We note that, so far, we have considered research interest for very few chemicals. Thus, we may yet determine that near-hits is a more appropriate means of quantifying research interest for our purposes.

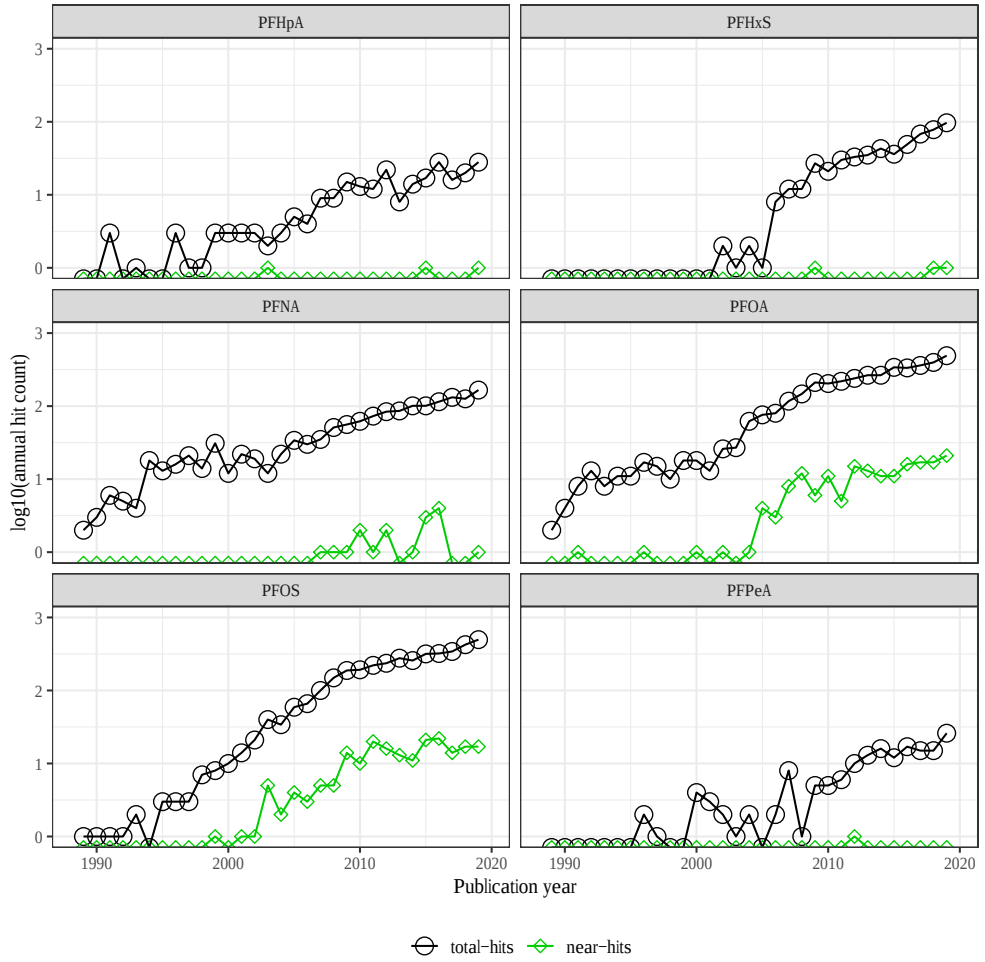

Figure 1: Graphs of time series of total-hits and near-hits counts for our PFAS over the publication range 1989–2019. Counts are presented on a logarithmic base-10 scale to assist comparisons between chemicals. Hits were obtained from Web of Science (Clarivate, 2020b).

Some PFAS show an early period of little interest, yet all have a generally increasing trend in total-hits for (at least) later years. We will exploit such features in formulating classification systems.

2.4 Classification Systems for Application to Total-Hits Series

Based on inspection of the total-hits time series in Figure 1, we propose two classification systems. Comparison of system results against PFAS regulatory history allows us to evaluate the system's ability to recognise emerging interest. Each classification system will use one or more of two tests, and their associated outcomes:

Test 1: Starting from 1989, is there a year in which the cumulative sum (cusum) of total-hits across consecutive publication years is at least 100?

Outcome 1: If yes, record the year of the earliest occurrence. Otherwise, record a non-result.

Test 2: Starting from 1989 and considering overlapping intervals of three consecutive years, is there an occurrence of at least 15 total-hits per year over an interval?

Outcome 2: If yes, for the first occurrence, record the final year of the interval. Otherwise, record a non-result.

We will consider the individual use of two classification rules to interpret these outcomes. We classify a chemical as of interest if:

Rule 1: Outcome 2 precedes any year of regulatory action.

Rule 2: At least one of Outcome 1 or Outcome 2 precedes any year of regulatory action. (We record the earliest of the outcomes.)

If the conditions for a rule are not satisfied, we classify a chemical as not of interest.

A classification system must balance correctly classifying as many CoI (true positives) and non-CoI (true negatives) as possible against controlling the misclassification of CoI and non-CoI (false negatives and false positives, respectively). False negatives conceal CoI, whilst false positives may cause a regulator to expend effort on unnecessary chemical assessments.

In the next section we apply our classification systems to the PFAS total-hits time series, and compare results against regulatory histories in Australia (and elsewhere, as necessary).

3 RESULTS AND DISCUSSION

Table 3 presents our classification results. We note that five PFAS — PFHpA, PFOA, PFOS, PFHxS, and PFNA — attracted regulatory interest. When selecting PFAS to consider early in this study, a lack of specific assessments suggested that PFHxS and PFNA held no particular concern for Australian regulators. As such, given the classifications made by Rules 1 and 2, PFHxS and PFNA would appear to be false positives. However, following the discovery of concern elsewhere, we emphasise our classifications of PFHxS and PFNA as true positives with bold type.

Test 1 and Test 2 are satisfied for all PFAS, and Outcome 1 precedes Outcome 2 for five cases. Outcome 2 for PFHpA exceeds the year in which concern was noted. Thus, Rule 1 regards PFHpA as a false negative. Also, Outcome 2 for PFPeA is greater than the year of the current status, leading Rule 1 to judge this chemical as a true negative. A question mark is appended to this judgement as we are unable to judge its future accuracy. This relates to our study's motivation; unrestricted chemicals can progress to being of concern relatively quickly. Rule 1 correctly recognises emerging interest in four of the five PFAS which attracted regulatory attention (but not PFHpA). Like Rule 1, Rule 2 also classifies PFPeA as a true negative. However, Rule 2 has better classification accuracy, anticipating emerging interest for all appropriate cases (the five true positives). The earliest value of Outcomes 1 and 2 for each individual PFAS shows the ability of our method to anticipate the concerns (or necessary actions) of a regulator, Australian or otherwise.

4 CONCLUSIONS AND RECOMMENDATIONS

We applied our classification systems to total-hits time series obtained for six PFAS. Three (five) were considered CoI according to Australian (international) regulatory attention. Classifications using Rule 1 returned one false negative, and anticipated the emergence of four CoI in advance of Australian regulatory concern. Classifications using Rule 2 anticipated the emergence of all five CoI. Encouraged by this, we intend to consider a greater range of chemicals, which must include some having a regulatory history. Experience suggests that searching for and interpreting relevant regulatory reports, drawn from various jurisdictions, may take some time. Studies such as ours will benefit from a consolidation of information that aids the discovery of regulatory histories.

We are currently applying our processes for obtaining and classifying research interest to further test cases, expecting this to inform improvements (Whyte, 2020). However, based on this study, we expect that investigation of certain areas may prove fruitful. Consider the data mining aspect. In our near-hits queries, our modifiers were informed by a non-specialist reading of a selection of articles and NICNAS reports. Contacts at NSW EPA have proposed more specific modifiers, and we are currently exploring their usefulness. We also recall the current system's limitation of requiring the manual processing of synonyms. To remedy this, we are investigating the successor to SciFinder®, SciFinder^{n}®, which promises to make future synonym extraction more efficient.

Our approach to the problem of classifying chemicals as CoI or otherwise will benefit from further refinement. Our framework allows certain choices: first, the type of test, and then, the value of the threshold employed (such as a cumulative sum of hits of 100). Here, we formulated tests by in-

Table 2: Selected details of the PFAS considered (from Chemical Abstracts Service (2019)).

CASRN	Acronym	Systematic name
375-85-9	PFHpA	Heptanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7,7-tridecafluoro-
355-46-4	PFHxS	1-Hexanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-
375-95-1	PFNA	Nonanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,9-heptadecafluoro-
335-67-1	PFOA	Octanoic acid, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluoro-
1763-23-1	PFOS	1-Octanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-
2706-90-3	PFPeA	Pentanoic acid, 2,2,3,3,4,4,5,5,5-nonafluoro-

Table 3: Regulatory histories for selected PFAS, test outcomes, and derived classifications. If NICNAS assessed a chemical as "noted" or "restricted", $^{+n}$ denotes an outcome n years in advance of the assessment year. Where a label is "unrestricted" or "no guidance", $^{+n}$ denotes an outcome n years in advance of 2020.

				Classification using:	
Acronym	Environmental status (year)	Outcome 1	Outcome 2	Rule 1 (O2)	Rule 2 (O1 or O2)
PFHpA	noted (2015[1], 2016[2])	2012^{+3}	2017	**false –**	true +
PFOA	noted (2015[3])	1999^{+16}	2004^{+11}	true +	true +
PFOS	restricted (2008[4], 2015[5])	2003^{+5}	2004^{+4}	true +	true +
PFHxS	no guidance (2020)	2011^{+9}	2011^{+9}	**true +**[6]	**true +**[6]
PFNA	no guidance (2020)	1998^{+22}	2006^{+14}	**true +**[7]	**true +**[7]
PFPeA	unrestricted (2015[8])	2016	2018	true – (?)	true – (?)

To explain categories used in the "Environmental status" column:
noted: "…having the potential to give rise to adverse outcomes for the environment and have been recommended for further risk management …",[2] or similar[1,3].
restricted: "…restricted to only essential uses, for which no suitable and less hazardous alternatives are available."[4,5]
unrestricted: "The use of the chemicals in this group is not subject to any specific national environmental regulations."[8]

[1]National Industrial Chemicals Notification and Assessment Scheme (2015a). [2]National Industrial Chemicals Notification and Assessment Scheme (2016). [3]National Industrial Chemicals Notification and Assessment Scheme (2015c). [4]National Industrial Chemicals Notification and Assessment Scheme (2013). [5]National Industrial Chemicals Notification and Assessment Scheme (2015b). [6]PFHxS and related compounds "…are likely as a result of their long-range environmental transport to lead to significant adverse human health and/or environmental effects such that global action is warranted …" (POPs Review Committee, 2019, Page 28). [7]It is anticipated that a draft toxicity assessment for PFNA will be released in 2020 (U.S. Environmental Protection Agency, 2019). [8]National Industrial Chemicals Notification and Assessment Scheme (2015d).

spection of the PFAS total-hits graphs, and evaluated the results for a small number of thresholds. It may be informative to adjust thresholds in a systematic manner and compare results.

We are currently exploring a larger set of time series so as to discover new types of tests able to discriminate between CoI and others. Two extensions to the methodology of this paper are under investigation. Both involve applying an initial test to each time series, determining the year of a test outcome, and excluding the data prior to this year from further consideration. Our first approach is to explore multi-condition tests, where we associate a test outcome with a time series only if the series satisfies all conditions. Early results indicate that multi-condition tests have a greater ability to discriminate between CoI and non-CoI chemicals compared to simple tests. The second approach creates 'rescaled' time series by setting the year of the initial test outcome to year zero (see Figure 2 for examples) so that time series are more directly comparable. Scrutiny of the rescaled time series may allow us to learn features particular to the research interest of CoI, which will assist us subsequently in classifying chemicals.

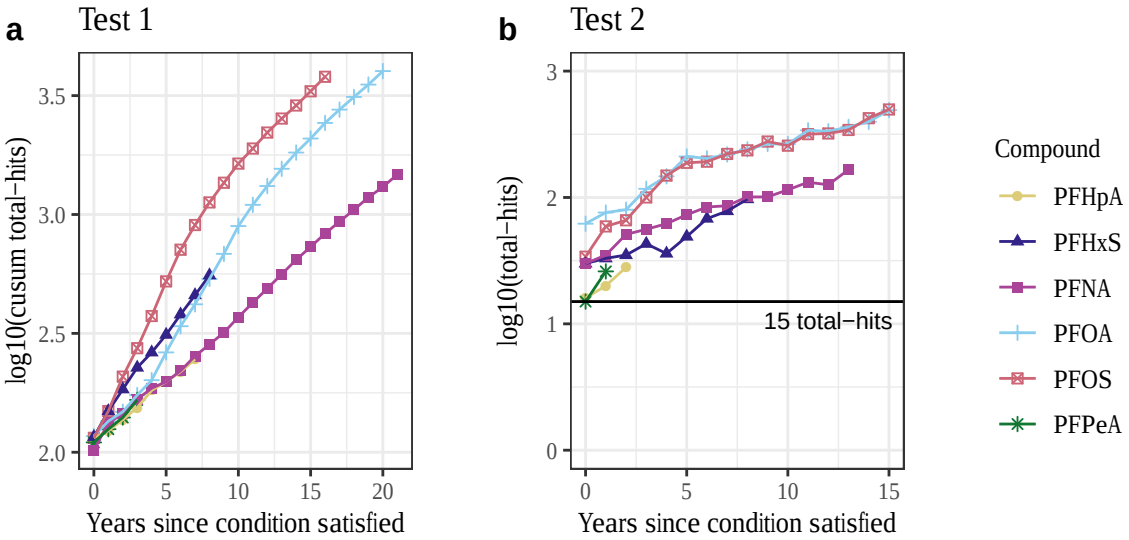

Figure 2: Rescaled total-hits time series for those which satisfy (a) Test 1, and (b) Test 2. The year in which a test is satisfied defines 'year zero' for the rescaled series; prior values are omitted.

Regulators seeking to proactively manage chemical risks may aspire to classifying many chemicals, and doing this in an ongoing manner so as to incorporate new knowledge. A substantially automated process will support such aspirations. Towards this, given a data set comparable to (but larger than) our test data here, we could improve our methodology by replacing our classification rules with an automated process, say, a decision tree classifier. To sketch the approach, suppose that each chemical and its research interest constitute a record, and the chemical's status (CoI or not CoI) acts as the record label. We would define a training subset of our records, associating each record therein with attributes: the outcomes associated with some number of tests. We would apply a learning algorithm to our training records, intending to produce a tree where each non-terminal node applies a binary split depending on a particular outcome's result/non-result value. Inadequate classifier performance requires us to review our tests. Adequate performance allows us to apply the classifier to the remaining records, again using our tests to assign values to the attributes for each record. Adequate performance allows us to proceed to consider the research interest of novel chemicals. We may choose to apply the tests and classifier annually so as to judge whether new research interest changes the classifications of these novel chemicals.

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